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NEWS
NEWS
                 "Ask CAS" for self-help around the clock
                New STN AnaVist pricing effective March 1, 2006
NEWS
        FEB 27
NEWS
        APR 04
                STN AnaVist $500 visualization usage credit offered
NEWS 5
        MAY 10
                CA/CAplus enhanced with 1900-1906 U.S. patent records
        MAY 11 KOREAPAT updates resume
NEWS 6
        MAY 19
NEWS
     7
                Derwent World Patents Index to be reloaded and enhanced
NEWS
        MAY 30
                IPC 8 Rolled-up Core codes added to CA/CAplus and
                 USPATFULL/USPAT2
NEWS 9
        MAY 30
                The F-Term thesaurus is now available in CA/CAplus
NEWS 10
        JUN 02
                The first reclassification of IPC codes now complete in
                 INPADOC
NEWS 11
        JUN 26
                TULSA/TULSA2 reloaded and enhanced with new search and
                 and display fields
NEWS 12
        JUN 28
                Price changes in full-text patent databases EPFULL and PCTFULL
NEWS 13
        JUl 11
                CHEMSAFE reloaded and enhanced
NEWS 14
        JUl 14
                FSTA enhanced with Japanese patents
NEWS 15
        JUl 19
                Coverage of Research Disclosure reinstated in DWPI
NEWS 16
        AUG 09
                INSPEC enhanced with 1898-1968 archive
NEWS 17 AUG 28
                ADISCTI Reloaded and Enhanced
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NEWS EXPRESS JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8
NEWS X25 X.25 communication option no longer available

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FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FILE 'REGISTRY' ENTERED AT 14:06:39 ON 29 AUG 2006

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STRUCTURE FILE UPDATES: 28 AUG 2006 HIGHEST RN 904961-01-9 DICTIONARY FILE UPDATES: 28 AUG 2006 HIGHEST RN 904961-01-9

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http://www.cas.org/ONLINE/UG/regprops.html

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=> e probucol/cn
                   PROBRIMIDE 200/CN
E1
                   PROBROMIDE 286/CN
E2
             1
             1 --> PROBUCOL/CN
E3
                   PROBUCOL DISUCCINATE/CN
E4
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E5
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E6
E7
             1
                   PROBURSIN TETRADECAPEPTIDE/CN
E8
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                   PROBUTYL DB 10/CN
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                   PROBUTYLIN/CN
E9
                   PROC (METHANOSPHAERA STADTMANAE STRAIN DSM 3091 GENE PROC)/C
E10
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E11
                   PROC) / CN
                   PROC (PASTEURELLA MULTOCIDA STRAIN IL1403 CLONE PM70 GENE PR
E12
             1
                   OC)/CN
=> e3
             1 PROBUCOL/CN
L1
=> d l1
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
L1
     23288-49-5 REGISTRY
RN
ED
     Entered STN: 16 Nov 1984
CN
     Phenol, 4,4'-[(1-methylethylidene)bis(thio)]bis[2,6-bis(1,1-dimethylethyl)-
      (9CI)
            (CA INDEX NAME)
OTHER CA INDEX NAMES:
     Acetone, bis(3,5-di-tert-butyl-4-hydroxyphenyl) mercaptole (8CI)
     Phenol, 4,4'-(isopropylidenedithio)bis[2,6-di-tert-butyl- (8CI)
OTHER NAMES:
     4,4'-(Isopropylidenedithio)bis[2,6-di-tert-butylphenol]
CN
CN
     Biphenabid
CN
     Bisbid
CN
     Bisphenabid
CN
     DH 581
CN
    Lipomal
CN
    Lorelco
CN
     Lurselle
    NSC 652160
CN
    NSC 86225
CN
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CN Panavir CN Phenbutol Probucol CN CN Sinlestal 3D CONCORD FS C31 H48 O2 S2 MF CI COM ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOSIS, LC STN Files: BIOTECHNO, CA, CABA, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMLIST, CIN, CSCHEM, DDFU, DRUGU, EMBASE, IFICDB, IFIPAT, IFIUDB, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE, MRCK*, PHAR, PROMT, PROUSDDR, PS, RTECS*, SCISEARCH, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL (*File contains numerically searchable property data) Other Sources: EINECS**, WHO (**Enter CHEMLIST File for up-to-date regulatory information)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1196 REFERENCES IN FILE CA (1907 TO DATE)
27 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1198 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> e5

L2

1 "PROBUCOL MONOSUCCINATE"/CN

=> d 12

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 216167-82-7 REGISTRY

ED Entered STN: 29 Dec 1998

CN Butanedioic acid, mono[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl] ester (9CI) (CA INDEX NAME)

OTHER NAMES:

CN AGI 1067

CN Probucol monosuccinate

CN Succinobucol

FS 3D CONCORD

MF C35 H52 O5 S2

CI COM

SR CA

LC STN Files: ADISINSIGHT, BIOSIS, CA, CAPLUS, CASREACT, EMBASE, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE, PROUSDDR, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL

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32 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

32 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 14.64 14.85

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 14:08:13 ON 29 AUG 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

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(FILE 'HOME' ENTERED AT 14:06:24 ON 29 AUG 2006)

FILE 'REGISTRY' ENTERED AT 14:06:39 ON 29 AUG 2006 E PROBUCOL/CN

L1 1 E3 L2 1 E5

FILE 'CAPLUS' ENTERED AT 14:08:13 ON 29 AUG 2006

=> 11

L3 1198 L1

=> save temp 13 probucols/a
ANSWER SET L3 HAS BEEN SAVED AS 'PROBUCOLS/A'

=> save temp 14 probucsucc/a
ANSWER SET L4 HAS BEEN SAVED AS 'PROBUCSUCC/A'

=> 12/prep

32 L2

3518443 PREP/RL

L5 7 L2/PREP

(L2 (L) PREP/RL)

=> base

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=> search base

676150 BASE

153063 BASES

L6 769298 BASE

(BASE OR BASES)

=> 15 and 16

L7 0 L5 AND L6

=> d 15 1-7 ti

- L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Process for preparing esters of probucol and derivatives thereof using acid anhydrides in the presence of DBU or DBN.
- L5 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Process for preparation of probucol derivatives
- L5 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Process of preparing esters and ethers of probucol and derivatives thereof
- L5 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Methods of reversing and preventing cardiovascular pathologies
- L5 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Probucol monoesters for increasing levels and improving functionality of plasma HDL cholesterol
- L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Process for preparing water-soluble probucol acyl esters for use as food antioxidants
- L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Preparation of phenolic compounds for the inhibition of the expression of VCAM-1

=> d 15 1-7 ti fbib abs

- L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Process for preparing esters of probucol and derivatives thereof using acid anhydrides in the presence of DBU or DBN.
- AN 2005:1170583 CAPLUS
- DN 143:440071
- TI Process for preparing esters of probucol and derivatives thereof using acid anhydrides in the presence of DBU or DBN.
- IN Weingarten, David M.
- PA Atherogenics, Inc., USA
- SO PCT Int. Appl., 68 pp. CODEN: PIXXD2
- DT Patent

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LΑ
     English
FAN.CNT 1
     PATENT NO.
                        KIND
                               DATE
                                           APPLICATION NO.
                                                                   DATE
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                                                                   -----
     WO 2005102323
                                           WO 2005-US13394
PΙ
                         A2
                                20051103
                                                                   20050420
     WO 2005102323
                         A3
                                20051215
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
            LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
            NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL,
             SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA,
             ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
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            EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
            RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
            MR, NE, SN, TD, TG
                                           US 2004-564267P
                                                                  20040420
     US 2005267187
                         Α1
                               20051201
                                           US 2005-111194
                                                                   20050420
                                           US 2004-564267P
                                                                  20040420
    MARPAT 143:440071
OS
GI
                          z^3
z^1
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WO 2005102985

AB Title compds. [I; Z1-Z4 = H, (substituted) alkyl; Z5, Z6 = (substituted) alkyl, alkenyl, aryl; Z5Z6 = atoms to form a carbocyclic ring; M = H, (substituted) (unsatd.) acyl; J = (substituted) (unsatd.) acyl], were prepared by reaction of I (M, J = H; other variables as above) with (substituted) (unsatd.) acyl halides, carboxylic acid anhydrides, or carboxylic acid esters in the presence of R1R3NCY(:NR4) (Y = R2, NR2R5; R1-R5 = (substituted) alkyl, alkenyl; R1R2, R3R4 = atoms to form rings). Thus, probucol, succinic anhydride, and DBU were stirred in MeCN at 50° for 1 h to give a mixture comprising probucol monosuccinate 49 weight%, probucol disuccinate 18 weight%, and probucol 33 weight%.

DATE

20040409

20040702

Ι

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L5
     ANSWER 2 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
TI
     Process for preparation of probucol derivatives
     2005:1103383 CAPLUS
ΑN
DN
     143:392944
     Process for preparation of probucol derivatives
ΤI
IN
     Jass, Paul Alan; Douglas, Jason Scott
PA
SO
     U.S. Pat. Appl. Publ., 5 pp.
     CODEN: USXXCO
DT
     Patent
LА
     English
FAN.CNT 1
                          KIND
                                 DATE
                                             APPLICATION NO.
     PATENT NO.
                          _ _ _ _
                                 20051013
                                             US 2004-821426
PΙ
     US 2005228192
                           A1
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A1

20051103

WO 2004-US21336

AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,

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NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
    TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
   AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
    EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
    SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
    SN, TD, TG
                                   US 2004-821426
                                                       A 20040409
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os MARPAT 143:392944

AΒ A method is described for the preparation of polymorphic forms of water-soluble derivs. of probucol compds. (Markush structure is given). Probucol was reacted with succinic anhydride to obtain mono-, and di-succinylated probucol derivs. which were separated and purified.

- ANSWER 3 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN L5
- Process of preparing esters and ethers of probucol and derivatives thereof TI
- 2004:610066 CAPLUS AN
- 141:156929 DN
- Process of preparing esters and ethers of probucol and derivatives thereof TI
- IN Weingarten, M. David; Sikorski, James A.
- PA Atherogenics, Inc., USA
- PCT Int. Appl., 136 pp. SO
- CODEN: PIXXD2
- DT Patent
- English LΑ

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	PAT	ENT 1	NO.			KIN	D	DATE			APP	LICAT	ION :	NO.		D	ATE	
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	WO :							2004										
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			LK,	LR,	LS,	LT,	LU,	LV,	MA,	•		, MK,	•	•	•			
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											US	2003-	4396	65P -		P 2	0030	113
	~ •	0-10						0004	0000		WO	2004-	0580	5		W 2	0040	113
	CA 2	2512	980			AA		2004	0729			2004-						
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	110 1	2004	2044) E		7.1		2004	1014		WU	2004 - 2004 -	7576	5 61		w 2	0040	113
	05 4	2004	2044	99		AI		2004	1014		TIC	2004-	1306	04 65 D		ע כם	0040	113
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	JP 2	2006!	5165	59		T2		2006	0706			2006-				_		
										US	2003-	4396	65P		P 2	0030	113	
											WO	2004-	US80.	5		W 2	0040	113

AB Probucol or a probucol derivative can be efficiently converted to a monoester or monoether of probucol (I) [wherein R1-R4 = H, (un)substituted alkyl; R5, R6 = each (un)substituted alkyl, alkenyl, or aryl; or R5 and R6 can come together to form a carbocyclic ring; X, Y = H, optionally substituted (un)saturated acyl having from 1 to 18 carbon atoms each optionally containing a

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polar or charged functionality] by reacting the free hydroxyl-containing probucol or a derivative thereof (by which is meant a probucol compound with at least one substituent that is different from that on the parent probucol mol. but which maintains the two free hydroxyl groups), i.e., I (X = Y = H; R1-R6 = same as above), with a Grignard reagent or a lithium reagent that produces a magnesium bromide or lithium salt of probucol or the probucol derivative. The probucol compound anion is then reacted with an ester or ether forming compound. Thus, in a dry 25 mL 3-neck round bottom flask fitted with a reflux condenser, nitrogen inlet, thermocouple and stir bar was charged probucol (0.25 g, 0.48 mmol) followed by 2.5 mL anhydrous toluene and then isopropylmagnesium chloride (0.51 mL, 2.0 M in THF) in 1 portion. The reaction was brought to room temperature and then succinic anhydride (0.25 g, 2.5 mmol) was added in 1 portion. After aging for 45 min, the reaction was slowly quenched with 1 N HCl and diluted with EtOAc. The biphasic reaction was then cooled to room temperature and the phases were separated to

an organic layer containing 60% probucol monosuccinate, 13% probucol disuccinate,

and 27% probucol according to HPLC anal.

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L5 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
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TI Methods of reversing and preventing cardiovascular pathologies

AN 2003:376540 CAPLUS

DN 138:362685

TI Methods of reversing and preventing cardiovascular pathologies

IN Glass, Mitchell; Tardif, Jean-Claude

PA Atherogenics, Inc., USA

SO PCT Int. Appl., 64 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

give

	PA	rent 1	NO.			KIN	D :	DATE			APPL	ICAT:	ION I	NO.		D	ATE	
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			•	•	•	•	•	•	•	•	•	MW, SL,	•	•	•	•	•	•
			•		•	UZ,	•	•	•	•	•	•	10,	114,	IN,	ıĸ,	11,	14,
		RW:										TZ, CH,						
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WO 2002-US37274
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                                        WO 2002-US37274
                                                               20021112
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OS MARPAT 138:362685

GI

AB The present invention is a method to increase the lumen diameter of a coronary blood vessel, that includes administering a lumen increasing amount of a compound of the formula I wherein x is defined as an integer between 1

Ι

L5 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI Probucol monoesters for increasing levels and improving functionality of plasma HDL cholesterol

and 4; or a pharmaceutically acceptable salt, ester or prodrug thereof.

AN 2002:849415 CAPLUS

DN 137:333157

TI Probucol monoesters for increasing levels and improving functionality of plasma HDL cholesterol

IN Luchoomun, Jayraz; Saxena, Uday; Sundell, Cynthia L.; Sikorski, James A.

PA Atherogenics, Inc., USA

SO PCT Int. Appl., 161 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

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	WO 20	020875	56		C2		2003	0320									
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			HR,														
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US 2001-283376P
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OS MARPAT 137:333157

AB It has been discovered that certain selected probucol monoesters, and their pharmaceutically acceptable salts or prodrugs, are useful for increasing circulating HDL cholesterol. These compds. may also improve HDL functionality by (a) increasing clearance of cholesteryl esters, (b) increasing HDL-particle affinity for hepatic cell surface receptors, or (c) increasing the half-life of apoAI-HDL. The pharmaceutical compns. comprise probucol monoesters alone or in combination with other agents, e.g, statins, IBAT inhibitors, MTP inhibitors, cholesterol absorption inhibitors, phytosterols, CETP inhibitors, fibric acid derivs., and antihypertensive agents. For example, mono[4-[[1-[[3,5-bis(1,1dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1dimethylethyl)phenyl]ester of pentanedioic acid, prepared from probucol and glutaric anhydride, elevated HDLc in hyperlipidemic hamster by 22% (average of 3 expts., range 5-44%), compared to untreated controls after 2 wk treatment at a dose of 150 mg/kg/day. LDLc was reduced by 29% on average, VLDL cholesterol by 42%, and triglycerides by 24%, compared to controls. The compound was well tolerated and all animals gained weight

- L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Process for preparing water-soluble probucol acyl esters for use as food antioxidants
- AN 2001:863541 CAPLUS
- DN 135:371524
- TI Process for preparing water-soluble probucol acyl esters for use as food antioxidants
- IN Jass, Paul Alan
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- SO U.S., 5 pp.

CODEN: USXXAM

- DT Patent
- LA English

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				US 2000-562657	20000502

OS CASREACT 135:371524; MARPAT 135:371524

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AB Water-soluble derivs. of probucol compds. [I; R1, R2 = alkyl, alkenyl, aryl; R3-R6 = C1-4 alkyl; X, Y = H, (un)saturated (un)substituted C1-8 acyl] (e.g., probucol mono- and disuccinate), useful as food antioxidants, are prepared by the reaction of a solution of a probucol compound (II) with an alkali metal hydroxide, alkali metal alkoxide (e.g., potassium tert-butoxide), alkylammonium alkoxide, alkylammonium hydroxide and mixts. forming an ammonium or an alkali metal salt of the probucol compound and reacting the salt with a carboxylic acid anhydride selected from succinic anhydride, glutaric anhydride, adipic anhydride, suberic anhydride, sebacic anhydride, azelaic anhydride, phthalic anhydride, and maleic anhydride.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2006 ACS on STN

TI Preparation of phenolic compounds for the inhibition of the expression of VCAM-1

AN 1998:761875 CAPLUS

DN 130:13646

TI Preparation of phenolic compounds for the inhibition of the expression of VCAM-1

IN Medford, Russell M.; Somers, Patricia K.; Hoong, Lee K.; Meng, Charles Q.

PA Atherogenics, Inc., USA

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		20023 66023		15		A1 B2		2002: 2003:			US	20	02-	1143	46			20020	402
	•••					22	•				US	19	97-	4702	0P		P	19970	514
														7921				19980	
	US	2002	1881:	18		A1		2002:	1212					3700 1152			ΑI	19990	
		6828				B2		2004											
														4702			P	19970	
														7921 3700				19980 19990	
	US	2002	19344	16		A1	:	2002	1219	•	US	20	02-	1143	51			20020	402
														4702 7921				19970	
														7921 3700				19980 19990	
	US	2005	09048	37		A1	:	2005	0428		US	20	03-	6477	66			20030	825
														4702 7921				19970 19980	
														7921 3700				19990	

				US	2002-60734	A1	20020130
US	2004138147	A1	20040715	US	2003-744763		20031223
US	7087645	B2	20060808				
				US	1997-47020P	P	19970514
				US	1998-79213	A1	19980514
				US	1999-370046	A2	19990806
				US	2000-191046P	P	20000321
				US	2001-815262	A2	20010321
		•		US	2001-36307	A1	20011025
US	2005171028	A1	20050804	US	2005-54644		20050208
				ະບຣ	2000-191046P	P	20000321
				ູບຣ	2001-815262	A1	20010321
US	2006189581	A1	20060824	US	2006-405798		20060418
				∮US	1997-47020P	P	19970514
				US	1998-79213	A1	19980514
				US	1999-370046	A2	19990806
				US	2000-191046P	P	20000321
				US	2001-815262	A2	20010321
	•			US	2001-36307	A1	20011025
				US	2003-744763	A1	20031223
AU	2006202461	A1	20060629	AU	2006-202461		20060609
				US	1997-47020P	P	19970514
				AU	2002-300328	Α3	20020730
MARE	DAM 120 12646						

OS MARPAT 130:13646

GI

$$R^{1}$$
 R
 R^{2}
 R^{4}
 R^{2}
 R^{4}

Title compds. [e.g., I; R = Z1Z2R5; R1,R2 = (un)substituted (cyclo)alkyl, -(hetero)aryl, etc.; R3,R4 = any group that does not otherwise adversely affect (sic) the desired properties of the mol. including H, halogen, or R1 (sic); R5 = (di)(alkyl)amino, alkyl, alkoxy(carbonyl), (hetero)aryl, etc.; Z1 = O SOO-2, NH, CH2; Z2 = bond, alkylene(oxy) aryleneoxy, etc.] were prepared Thus, 4-(BrCH2)C6H4CH2CO2H was thioetherified by 4-mercapto-2,6-di-tert-butylphenol to give I [R = SCH2C6H4(CH2CO2H)-4, R1 = R2 = CMe3, R3 = R4 = H]. Data for biol. activity of I were given.

```
=> phenol
```

243606 PHENOL

116016 PHENOLS

L8 302679 PHENOL

(PHENOL OR PHENOLS)

=> bisphenolo

0 BISPHENOLO

L9 0 BISPHENOLO

=> bisphenol

71469 BISPHENOL

4778 BISPHENOLS

L10 72881 BISPHENOL

(BISPHENOL OR BISPHENOLS)

=> grignard

43179 GRIGNARD

638 GRIGNARDS

L11 43342 GRIGNARD

(GRIGNARD OR GRIGNARDS)

=> 110 and 111

L12 32 L10 AND L11

=> 110(1)111

L13 13 L10(L)L11

=> d l13 1-13 ti

L13 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN

- TI Advances in nanocontact molding for the patterning of polythiophene
- L13 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Manufacture of a N-heterocyclic-substituted poly(aryl ether sulfone)
- L13 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Manufacture of functionalized polyaryl ether sulfones via bromination
- L13 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Dialkyl titanium complexes that contain a sulfur-linked bis(phenolato) ligand: the structure of an olefin polymerization catalyst precursor
- L13 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI New bisphenols with silylene fragments: synthesis and spectra
- L13 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Photochromic heterocyclic fused indenonaphthopyrans
- L13 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Knots for Molecular Strings of Beads
- L13 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Thermal printing materials
- L13 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI 3,3-Bis(2,2-diphenylvinyl)phthalides as leuco dyes and recording materials containing them
- L13 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Catalysts for manufacture of olefin random copolymers
- L13 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Recording material
- L13 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Products of the thermal degradation of the adduct of bisphenol A diglycidyl ether and p,p'-diaminodiphenylmethane
- L13 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Linear polycondensates of triazine monomers

=> monosub?

L14 10656 MONOSUB?

=> 110 and 114

L15 20 L10 AND L14

=> 112 and 115

=> d l15 10-20 ti

- L15 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Thermotropic liquid-crystalline aromatic polyesters
- L15 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI A comparison of spin relaxation and local motion between symmetrically and asymmetrically ring-substituted bisphenol units in dissolved polycarbonates
- L15 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Poly(2-aminoalkyl)polyamines
- L15 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Correlation analysis of polycondensation processes
- L15 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Oxidation of bisphenols. II. Some compounds related to galvinoxyl
- L15 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Synthesis of mixed phosphites and study of their inhibiting action against the oxidative thermal aging of low-density polyethylene
- L15 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Synthesis and study of sterically hindered bisphenols as light stabilizers of polyethylene
- L15 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Carboxy copolymers prepared in 1,2-epoxy compounds
- L15 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Lubricating oil compositions
- L15 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Stabilizing agents to inhibit the degradation of poly- α -olefins by light and heat
- L15 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Derivatives of triphenylphosphine and triphenylphosphine oxide

=> d 115 16 ti fbib abs

- L15 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Synthesis and study of sterically hindered bisphenols as light stabilizers of polyethylene
- AN 1978:510890 CAPLUS
- DN 89:110890
- TI Synthesis and study of sterically hindered bisphenols as light stabilizers of polyethylene
- AU Naumova, S. F.; Balykina, M. V.; Akulich, Z. I.; Velikanova, L. V.; Bolbotunova, T. N.
- CS Inst. Fiz.-Org. Khim., Minsk, USSR
- SO Doklady Akademii Nauk BSSR (1978), 22(5), 437-9 CODEN: DBLRAC; ISSN: 0002-354X
- DT Journal
- LA Russian

GΙ

OH OH OH OH OH OH
$$CH_2$$
 OH CH_2 CMe_2 CMe_2

The title bisphenols I [67013-77-8] and II [67066-61-9] were prepared by alkylation with 2-cyclohexen-1-one [930-68-7] of m-cresol [108-39-4] and 2,2-bis(4-hydroxyphenyl)propane [80-05-7], resp., and condensation of the resulting monosubstituted products with HCHO [50-00-0]. Tests in low-d. polyethylene [9002-88-4] indicated that I and II were as effective light stabilizers as Benzon OA (2-hydroxy-4-alkoxybenzophenone). I and II, by being solid (m.p. 50-5 and 65-70°, resp.), offered advantages over liquid Benzon OA.

ΙI

=> d his

(FILE 'HOME' ENTERED AT 14:06:24 ON 29 AUG 2006)

OH

FILE 'REGISTRY' ENTERED AT 14:06:39 ON 29 AUG 2006 E PROBUCOL/CN

L1 1 E3 L2 1 E5

FILE 'CAPLUS' ENTERED AT 14:08:13 ON 29 AUG 2006

L3 1198 L1

SAVE TEMP L3 PROBUCOLS/A

L4 32 L2

SAVE TEMP L4 PROBUCSUCC/A

L5 7 L2/PREP

L6 769298 SEARCH BASE

OH

L7 0 L5 AND L6

L8 302679 PHENOL

L9 0 BISPHENOLO

L10 72881 BISPHENOL

L11 43342 GRIGNARD

L12 32 L10 AND L11 L13 13 L10(L)L11

L14 10656 MONOSUB?

L15 20 L10 AND L14

16 0 L12 AND L15

=> save temp all mysrch/l

L# LIST L1-L16 HAS BEEN SAVED AS 'MYSRCH/L'

=> d 117

LΑ

German

```
ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
L17
     2004:610066 CAPLUS
AN
DN
     141:156929
TI
     Process of preparing esters and ethers of probucol and derivatives thereof
IN
     Weingarten, M. David; Sikorski, James A.
     Atherogenics, Inc., USA
PA
     PCT Int. Appl., 136 pp.
so
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                       KIND
                               DATE
                                          APPLICATION NO.
     -----
                         ----
                                ------
                                            -----
                                                                   _____
PΙ
     WO 2004062622
                         A2
                                20040729
                                           WO 2004-US805
                                                                  20040113
     WO 2004062622
                         A3
                                20041202
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ
                                20040729
                                          AU 2004-204824
     AU 2004204824
                         A1
     CA 2512980
                                20040729
                                           CA 2004-2512980
                         AA
                                                                  20040113
     US 2004204485
                         Α1
                                20041014
                                           US 2004-757664
                                                                  20040113
     EP 1594824
                                20051116
                                          EP 2004-701812
                         A2
                                                                  20040113
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
                               20051220
                                          BR 2004-6738
     BR 2004006738
                         Α
     CN 1759084
                         Α
                                20060412
                                           CN 2004-80006265
                                                                  20040113
     JP 2006516569
                         T2
                                20060706
                                           JP 2006-500935
                                                                  20040113
PRAI US 2003-439665P
                         Р
                               20030113
     WO 2004-US805
                         W
                               20040113
    MARPAT 141:156929
OS
=> 18 (1) 111
          364 L8 (L) L11
L18
=> butoxide
         12148 BUTOXIDE
          259 BUTOXIDES
L19
         12253 BUTOXIDE
                 (BUTOXIDE OR BUTOXIDES)
=> 118 (1) 119
            0 L18 (L) L19
=> 118 and 119
L21
            1 L18 AND L19
=> d 121
L21
    ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     1979:186581 CAPLUS
DN
     90:186581
TI
    Hydroxyalkyl- and oxoalkyl-substituted phenols
IN
    Althuis, Thomas Henry; Harbert, Charles Armon; Johnson, Michael Ross;
    Melvin, Lawrence Sherman, Jr.
    Pfizer Inc., USA
PA
SO
    Ger. Offen., 54 pp.
    CODEN: GWXXBX
DT
    Patent
```

FAN.	CNT 1				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	DE 2839884	A1	19790315	DE 1978-2839884	19780913
	DE 2839884	C2	19821125		
	US 4283569	Α	19810811	US 1977-832868	19770913
	JP 54048728	A2	19790417	JP 1978-111620	19780911
	JP 56043450	B4	19811013		
	BE 870402	A1	19790312	BE 1978-190417	19780912
	DK 7804011	Α	19790314	DK 1978-4011	19780912
	NL 7809270	Α	19790315	NL 1978-9270	19780912
	FR 2402640	A1	19790406	FR 1978-26122	19780912
	FR 2402640	B1	19810227		
	GB 2005257	Α	19790419	GB 1978-36417	19780912
	GB 2005257	B2	19820526		
	US 4284829	Α	19810818	US 1978-972595	19781222
	JP 56045437	A2	19810425	JP 1980-85032	19800623
	JP 59011571	B4	19840316		
	NL 8007036	Α	19810331	NL 1980-7036	19801224
PRAI	US 1977-832868	Α	19770913		
os	CASREACT 90:186581				

=>

A single name cannot be used for two saved items at the same time. Enter "Y" if you wish to replace the current saved name with a new definition. Enter "N" if the current saved definition must be preserved. You may then reenter the SAVE command with a different saved name. Enter "DISPLAY SAVED" at an arrow prompt (=>) to see a list of your currently defined saved names.

REPLACE OLD DEFINITION? Y/(N):y

L# LIST L1-L21 HAS BEEN SAVED AS 'MYSRCH/L'

=> logoff hold

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	87.16	102.01
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-6.00	-6.00

SESSION WILL BE HELD FOR 60 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 14:47:34 ON 29 AUG 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

Welcome to STN International

Web Page URLs for STN Seminar Schedule - N. America NEWS

"Ask CAS" for self-help around the clock NEWS

3 FEB 27 New STN AnaVist pricing effective March 1, 2006 NEWS

^{=&}gt; save temp all mysrch/l

^{&#}x27;MYSRCH/L' IN USE

NEWS 4 APR 04 STN AnaVist \$500 visualization usage credit offered NEWS 5 MAY 10 CA/Caplus enhanced with 1900-1906 U.S. patent records NEWS 6 MAY 11 KOREAPAT updates resume NEWS 7 MAY 19 Derwent World Patents Index to be reloaded and enhanced NEWS 8 MAY 30 IPC 8 Rolled-up Core codes added to CA/CAplus and USPATFULL/USPAT2 NEWS 9 MAY 30 The F-Term thesaurus is now available in CA/CAplus NEWS 10 JUN 02 The first reclassification of IPC codes now complete in INPADOC NEWS 11 JUN 26 TULSA/TULSA2 reloaded and enhanced with new search and and display fields NEWS 12 JUN 28 Price changes in full-text patent databases EPFULL and PCTFULL NEWS 13 JUL 11 CHEMSAFE reloaded and enhanced NEWS 14 JUl 14 FSTA enhanced with Japanese patents NEWS 15 JUl 19 Coverage of Research Disclosure reinstated in DWPI NEWS 16 AUG 09 INSPEC enhanced with 1898-1968 archive

NEWS 17 AUG 28 ADISCTI Reloaded and Enhanced

NEWS EXPRESS JUNE 30 CURRENT WINDOWS VERSION IS V8.01b, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP). AND CURRENT DISCOVER FILE IS DATED 26 JUNE 2006.

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Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus

FILE 'HOME' ENTERED AT 07:14:09 ON 30 AUG 2006

=> file reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.42 0.42

FILE 'REGISTRY' ENTERED AT 07:15:12 ON 30 AUG 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 AUG 2006 HIGHEST RN 904961-01-9 DICTIONARY FILE UPDATES: 28 AUG 2006 HIGHEST RN 904961-01-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of

experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10757664\10757664 probucol deriv core.str

chain nodes : 7 8 9 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 ring nodes : 1 2 3 4 5 6 10 11 12 13 14 15 chain bonds : 1-28 2-33 3-24 5-7 7-8 8-9 8-37 8-38 9-10 12-16 13-32 14-20 16-17 16-18 16-19 20-21 20-22 20-23 24-25 24-26 24-27 28-29 28-30 28-31 32-34 34-35 34-36 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15 exact/norm bonds : 2-33 5-7 7-8 8-9 9-10 13-32 32-34 34-36 exact bonds : 1-28 3-24 8-37 8-38 12-16 14-20 16-17 16-18 16-19 20-21 20-22 20-23 24-25 24-26 24-27 28-29 28-30 28-31 34-35 normalized bonds :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> serch 11 sss sam

COMBINATION OF STRUCTURE AND TEXT TERMS NOT VALID

The query entered contains both search terms created by

structure-building or screen commands and text search terms. L#s

created via the STRUCTURE or SCREEN commands must be searched in the

structures files separately from text terms or profiles. The L#

answer sets from structure searches can be used in crossover searches

and can be combined with text terms.

=> search 11 sss sam
SAMPLE SEARCH INITIATED 07:15:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 15 TO ITERATE

100.0% PROCESSED 15 ITERATIONS 3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 68 TO 532 PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> d scan

L2 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

. .

MF C35 H54 O4 S2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):3

L2 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 4-[[hydroxy(2-hydroxyphenoxy)phosphinyl]oxy]-,
4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl ester (9CI)
MF C41 H59 O8 P S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L2 3 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2-Butenedioic acid (2Z)-, mono[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl]
ester (9CI)

MF C35 H50 O5 S2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> search l1 sss full FULL SEARCH INITIATED 07:16:32 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -

260 TO ITERATE

41 ANSWERS

100.0% PROCESSED 260 ITERATIONS

SEARCH TIME: 00.00.02

L3 41 SEA SSS FUL L1

=> d scan

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-Glucitol, 1-deoxy-1-(methylamino)-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl butanedioate (salt) (9CI)

MF C35 H52 O5 S2 . C7 H17 N O5

CM 1

CM 2

Absolute stereochemistry.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):41

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Propanoic acid, 3-hydroxy-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenylester (9CI)

MF C34 H52 O4 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Acetic acid, [2-[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-

1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenoxy]-2-oxoethoxy]- (9CI) MF C35 H52 O6 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanedioic acid, 2,2-dimethyl-, 4-[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl]
ester (9CI)

MF C37 H56 O5 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C36 H54 N4 O3 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Phenol, 4-[[1-[[4-(acetyloxy)-3,5-bis(1,1-dimethylethyl)phenyl]thio]-1methylethyl]thio]-2,6-bis(1,1-dimethylethyl)- (9CI)

MF C33 H50 O3 S2

- L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- IN Butanoic acid, 4-bromo-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl
 ester (9CI)
- MF C35 H53 Br O3 S2

$$t-Bu$$
 $S-C-S$
 O
 $O-C-(CH2)3-Br$
 $t-Bu$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- IN Butanoic acid, 4-(sulfooxy)-, 1-[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl]
 ester, monosodium salt (9CI)
- MF C35 H54 O7 S3 . Na

Na

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 2H-Isoindole-2-acetic acid, 1,3-dihydro-1,3-dioxo-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl ester (9CI)

MF C41 H53 N O5 S2

$$\begin{array}{c|c}
O & & & & & & & & \\
N & & & & & & & \\
O & & & & & & \\
O & & & & & & \\
O & & & & & \\
O & & & & & \\
\end{array}$$

$$\begin{array}{c}
Me \\
S & & & & \\
Me \\
OH \\
\end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN L-Arginine, N2-[4-[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenoxy]1,4-dioxobutyl]- (9CI)

MF C41 H64 N4 O6 S2

Absolute stereochemistry.

 \sim NH₂

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-Glucitol, 1-deoxy-1-(methylamino)-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl heptanedioate (salt) (9CI)

MF C38 H58 O5 S2 . C7 H17 N O5

CM 1

CM 2

Absolute stereochemistry.

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 1-Piperazineacetic acid, 4-[3-(nitrooxy)propyl]-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl ester (9CI)

MF C40 H63 N3 O6 S2

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Pentanedioic acid, hexafluoro-, mono[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl]
ester (9CI)

MF C36 H48 F6 O5 S2

$$t-Bu$$
 $S-C-S$
 O
 $O-C-(CF_2)_3-CO_2H$
 $t-Bu$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C35 H50 O5 S2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanedioic acid, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl methyl ester (9CI)

MF C36 H54 O5 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- MF C36 H54 O5 S2
- CI COM

$$t-Bu$$
 $S-C$
 Me
 $O-C-(CH2)3-CO2H
 $t-Bu$$

- L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- MF C38 H58 O5 S2
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- IN Butanoic acid, 4-(nitrooxy)-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenylester (9CI)
- MF C35 H53 N O6 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- IN Pentanedioic acid, 2-hydroxy-, 1-[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-

 $\label{lem:hydroxyphenyl} $$ hydroxyphenyl] thio] -1-methylethyl] thio] -2,6-bis(1,1-dimethylethyl) phenyl] ester, (2R) - (9CI)$

MF C36 H54 O6 S2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C40 H62 O5 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 4-amino-4-oxo-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenylester (9CI)

MF C35 H53 N O4 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Glycine, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl ester (9CI)
MF C33 H51 N O3 S2

$$t-Bu$$
 $S-C-S$
 Me
 $O-C-CH_2-NH_2$
 $t-Bu$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-Glucitol, 1-deoxy-1-(methylamino)-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl hexanedioate (salt) (9CI)

MF C37 H56 O5 S2 . C7 H17 N O5

CM 1

CM 2

Absolute stereochemistry.

- L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- IN Propanedioic acid, mono[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl]
 ester (9CI)
- MF C34 H50 O5 S2
- CI COM

- L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- IN 2-Butenedioic acid, 2-(acetyloxy)-, 4-[4-[[1-[[3,5-bis(1,1-dimethylethyl)4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1dimethylethyl)phenyl] ester (9CI)
- MF C37 H52 O7 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- MF C41 H64 O5 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
- IN Butanoic acid, 4-(sulfooxy)-, 1-[4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl]
 ester (9CI)
- MF C35 H54 O7 S3
- CI COM

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 4-hydroxy-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl
ester (9CI)

MF C35 H54 O4 S2

$$t-Bu$$
 $S-C-S$
 O
 $O-C-(CH2)3-OH$
 $t-Bu$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-Glucitol, 1-deoxy-1-(methylamino)-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl pentanedioate (salt) (9CI)

MF C36 H54 O5 S2 . C7 H17 N O5

CM 1

$$t-Bu$$
 $S-C-S$
 O
 $O-C-(CH2)3-CO2H
 $t-Bu$$

CM 2

Absolute stereochemistry.

1

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 3,4-dihydroxy-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenylester (9CI)

MF C35 H54 O5 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-Aspartic acid, N-(phenylacetyl)-, 4-[4-[[1-[[3,5-bis(1,1-dimethylethyl)4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1dimethylethyl)phenyl] ester (9CI)

MF C43 H59 N O6 S2

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C39 H60 O5 S2

$$t-Bu$$
 $S-C-S$
 O
 $O-C-(CH2)6-CO2H
 $t-Bu$$

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 4-hydroxy-3,3-dimethyl-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl
ester (9CI)

MF C37 H58 O4 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C35 H52 O5 S2

CI COM

$$t-Bu$$
 $S-C-S$
 O
 $C-CH_2-CH_2-CO_2H$
 $t-Bu$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN D-Glucitol, 1-deoxy-1-(methylamino)-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl propanedioate (salt) (9CI)

MF C34 H50 O5 S2 . C7 H17 N O5

CM 1

Absolute stereochemistry.

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Pentanoic acid, 5-hydroxy-, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenylester (9CI)

MF C36 H56 O4 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C33 H48 O5 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

MF C37 H56 O5 S2

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Butanoic acid, 4-[[hydroxy(2-hydroxyphenoxy)phosphinyl]oxy]-,
4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl ester (9CI)

MF C41 H59 O8 P S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 41 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Pentanedioic acid, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl methyl ester (9CI)
MF C37 H56 O5 S2

$$t-Bu$$
 $S-C-S$
 Me
 $O-C-(CH2)3-C-OMe$
 $t-Bu$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

Uploading C:\Documents and Settings\PZucker\My Documents\Examination Auxillary files\10757664\10757664 probucol amino sub core.str

chain nodes : 7 8 9 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 ring nodes : 1 2 3 4 5 6 10 11 12 13 14 15 chain bonds : 1-28 2-33 3-24 5-7 7-8 8-9 8-37 8-38 9-10 12-16 13-32 14-20 16-17 16-18 16-19 20-21 20-22 20-23 24-25 24-26 24-27 28-29 28-30 28-31 32-34 34-35 34-36 35-39 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15 exact/norm bonds : 2-33 5-7 7-8 8-9 9-10 13-32 32-34 34-36 35-39 exact bonds : 1-28 3-24 8-37 8-38 12-16 14-20 16-17 16-18 16-19 20-21 20-22 20-23 24-25 24-26 24-27 28-29 28-30 28-31 34-35 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 39:CLASS 39:CLASS

L4 STRUCTURE UPLOADED

=> d 14 L4 HAS NO ANSWERS L4 STR

Structure attributes must be viewed using STN Express query preparation.

=> search 14 sss sam

SAMPLE SEARCH INITIATED 07:20:32 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 15 TO ITERATE

100.0% PROCESSED 15 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 68 TO 532
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> search 14 sss full

FULL SEARCH INITIATED 07:23:53 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 260 TO ITERATE

100.0% PROCESSED 260 ITERATIONS 1 ANSWERS

SEARCH TIME: 00.00.04

L6 1 SEA SSS FUL L4

=> d scan

L6 1 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Glycine, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl ester (9CI)

MF C33 H51 N O3 S2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d 16

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 216167-93-0 REGISTRY

ED Entered STN: 29 Dec 1998

CN Glycine, 4-[[1-[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]thio]-1methylethyl]thio]-2,6-bis(1,1-dimethylethyl)phenyl ester (9CI) (CA INDEX
NAME)

FS 3D CONCORD

MF C33 H51 N O3 S2

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL

$$t-Bu$$
 $S-C-S$
 0
 0
 $C-CH_2-NH_2$
 $t-Bu$
 $t-Bu$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)

5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 341.50 341.92

FULL ESTIMATED COST

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=> 16/prep

5 L6

3519114 PREP/RL L7 1 L6/PREP

(L6 (L) PREP/RL)

=> d 17 ti fbib abs

L7 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

- TI Preparation of phenolic compounds for the inhibition of the expression of VCAM-1
- AN 1998:761875 CAPLUS
- DN 130:13646

غ (قب**ي** (ھ

- TI Preparation of phenolic compounds for the inhibition of the expression of VCAM-1
- IN Medford, Russell M.; Somers, Patricia K.; Hoong, Lee K.; Meng, Charles Q.
- PA Atherogenics, Inc., USA
- SO PCT Int. Appl., 109 pp. CODEN: PIXXD2
- DT Patent

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                                           APPLICATION NO.
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	мас	ነገገር ጥልባ	13644	5					•	ΑU	2002-300328	A3	20020730

$$R^{1}$$
 R^{1}
 R^{2}
 R^{4}
 R^{2}
 R^{4}

Title compds. [e.g., I; R = Z1Z2R5; R1,R2 = (un)substituted (cyclo)alkyl, -(hetero)aryl, etc.; R3,R4 = any group that does not otherwise adversely affect (sic) the desired properties of the mol. including H, halogen, or R1 (sic); R5 = (di)(alkyl)amino, alkyl, alkoxy(carbonyl), (hetero)aryl, etc.; Z1 = O SOO-2, NH, CH2; Z2 = bond, alkylene(oxy) aryleneoxy, etc.] were prepared Thus, 4-(BrCH2)C6H4CH2CO2H was thioetherified by 4-mercapto-2,6-di-tert-butylphenol to give I [R = SCH2C6H4(CH2CO2H)-4, R1 = R2 = CMe3, R3 = R4 = H]. Data for biol. activity of I were given.

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L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

TI Probucol-related compounds and methods for treating diabetic vascular diseases

L8 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

TI Probucol-related compounds and methods for treating transplant rejection

L8 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

TI Probucol derivatives and methods for treating transplant rejection

L8 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

TI Methods and compositions to lower plasma cholesterol levels

L8 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

TI Preparation of phenolic compounds for the inhibition of the expression of VCAM-1

=> d 18 1-5 ti fbib abs

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

TI Probucol-related compounds and methods for treating diabetic vascular diseases

AN 2006:53906 CAPLUS

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TI Probucol-related compounds and methods for treating diabetic vascular diseases

IN Sundell, Cynthia L.; Kunsch, Charles

PA Atherogenics, Inc., USA

SO PCT Int. Appl., 83 pp. CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

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              KZ, MD, RU, TJ, TM
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 R1
               Me
                             OYZ
HO
      R<sup>2</sup>
                       R4
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AB
     The invention discloses compns. and methods of use of compds. I [Y = bond,
     C(0); R1-R4 = H, OH, alkyl, aryl, etc.; Z = alkyl, alkenyl, alkynyl, aryl,
     etc.], and pharmaceutically acceptable salts thereof, for the treatment of
     diabetic vascular diseases such as diabetic neuropathy, nephropathy, and
     retinopathy. Compds. of the invention include e.g. AGIX-4207.
     ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
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     Probucol-related compounds and methods for treating transplant rejection
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     Probucol-related compounds and methods for treating transplant rejection
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     Glass, Mitchell; Edwards, David B.
IN
     Atherogenics, Inc., USA
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     PCT Int. Appl., 87 pp.
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     PATENT NO.
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              PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
              UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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     The invention discloses the use of probucol-related compds. (Markush
     included), and pharmaceutically acceptable salts thereof, alone or in
     combination, for the treatment of transplant rejection.
    ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
     Probucol derivatives and methods for treating transplant rejection
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    Atherogenics, Onc., USA
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			BG, BR, BY, CA, CH,	CN, CU, CZ, DE,
	DK, EE, ES,	, FI, GB, GE, GH,	GM, GW, HU, ID, IL,	IS, JP, KE, KG,
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			SG, SI, SK, SL, TJ,	TM, TR, TT, UA,
		, VN, YU, ZW		
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			WO 1998-US9773	
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								WO	1998-	US97	73		W	19980	0514
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								US	1997-	47020	PΩ		P		
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The invention discloses the use of I [R1-R4 = H, OH, C1-10 alkyl, aryl, AB heteroaryl, etc.; Y = bond, C(0); Z = C1-10 alkyl, C2-10 alkenyl, C2-10 alkynyl, etc.], and pharmaceutically acceptable salts thereof, alone or in combination, for the treatment of transplant rejection. Preparation of I [R1-R4 = tert-butyl; YZ = (CH2)3COOH] from probucol which was evaluated in a graft arteriopathy model and Me 4-chlorobutyrate is described.

L8 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

TI Methods and compositions to lower plasma cholesterol levels

AN 2000:335659 CAPLUS

DN 132:343330

TΙ Methods and compositions to lower plasma cholesterol levels

Medford, Russell M.; Saxena, Uday IN

Atherogenics, Inc., USA PA

SO PCT Int. Appl., 50 pp.

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A method for determining whether a compound binds to a lipoprotein, e.g. LDL or VLDL, in a manner which will lower plasma cholesterol is provided that includes assessing the ability of the compound to form a complex with the lipoprotein, e.g., LDL or VLDL, and then determining whether the newly formed complex causes a change in the structure of apoB-100 that results in

increased binding affinity to the LDL receptor. Also disclosed is a method for lowering cholesterol in a host in need thereof, including a human, that includes the administration of an effective amount of a compound which binds to cholesterol-carrying lipoprotein (e.g. LDL or VLDL) in a manner that alters the three dimensional configuration of the lipoprotein and increases the binding affinity of the apoB-100 protein to the LDL receptor, including those on the surface of a hepatic cell.

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MAR	PAT 130:1	3646	5								

$$R^1$$
 R^3
 R^4
 R^2
 R^4

Title compds. [e.g., I; R = Z1Z2R5; R1,R2 = (un) substituted (cyclo) alkyl, -(hetero) aryl, etc.; R3,R4 = any group that does not otherwise adversely affect (sic) the desired properties of the mol. including H, halogen, or R1 (sic); R5 = (di) (alkyl) amino, alkyl, alkoxy(carbonyl), (hetero) aryl, etc.; Z1 = O SOO-2, NH, CH2; Z2 = bond, alkylene(oxy) aryleneoxy, etc.] were prepared Thus, 4-(BrCH2) C6H4CH2CO2H was thioetherified by 4-mercapto-2,6-di-tert-butylphenol to give I [R = SCH2C6H4 (CH2CO2H)-4, R1 = R2 = CMe3, R3 = R4 = H]. Data for biol. activity of I were given.

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NEWS 14 JUl 14 FSTA enhanced with Japanese patents
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NEWS 15 JUl 19 Coverage of Research Disclosure reinstated in DWPI

NEWS 16 AUG 09 INSPEC enhanced with 1898-1968 archive

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```
=> e Phenol,
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4-((1-((4-(acetyloxy)-3,5-bis(1,1-dimethylethyl)phenyl)thio)-1-methylethyl)thio)-2,6-bis(1,1-dimethylethyl)-/cn

E1 PHENOL, 4-((1-((4-(4-AMINOBUTOXY)-3,5-DIMETHYLPHENYL)THIO)-1
-METHYLETHYL)THIO)-2,6-BIS(1,1-DIMETHYLETHYL)-/CN

PHENOL, 4-((1-((4-(4-AMINOBUTOXY)PHENYL)THIO)-1-METHYLETHYL)
THIO)-2,6-BIS(1,1-DIMETHYLETHYL)-/CN

E3 1 --> PHENOL, 4-((1-((4-(ACETYLOXY)-3,5-BIS(1,1-DIMETHYLETHYL)PHEN

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YL) THIO) -1-METHYLETHYL) THIO) -2,6-BIS(1,1-DIMETHYLETHYL) -/CN
E4
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=> d l1

- L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
- RN 729583-53-3 REGISTRY
- ED Entered STN: 21 Aug 2004
- CN Phenol, 4-[[1-[[4-(acetyloxy)-3,5-bis(1,1-dimethylethyl)phenyl]thio]-1-methylethyl]thio]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)
- FS 3D CONCORD
- MF C33 H50 O3 S2
- SR CA
- LC STN Files: CA, CAPLUS, USPATFULL

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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=> **11**

L22 L1

=> d 12 1-2 ti fbib abs

- ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN L2
- Process for preparing esters of probucol and derivatives thereof using ΤI acid anhydrides in the presence of DBU or DBN.
- 2005:1170583 CAPLUS AN
- DN 143:440071
- Process for preparing esters of probucol and derivatives thereof using ΤI acid anhydrides in the presence of DBU or DBN.
- Weingarten, David M. TN
- PΑ Atherogenics, Inc., USA
- PCT Int. Appl., 68 pp. SO CODEN: PIXXD2
- Patent DT
- LA English

FAN.		1																
					KIND		DATE		APPLICATION NO.					DATE				
PI	WO 2005102323 WO 2005102323			A2 20051103			WO 2005-US13394				20050420							
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MARPAT 143:440071 OS

GI

$$Z^1$$
 Z^2
 Z^3
 Z^5
 Z^6
 Z^4
 Z^3
 Z^4
 Z^4

AB Title compds. [I; Z1-Z4 = H, (substituted) alkyl; Z5, Z6 = (substituted) alkyl, alkenyl, aryl; Z5Z6 = atoms to form a carbocyclic ring; M = H, (substituted) (unsatd.) acyl; J = (substituted) (unsatd.) acyl], were prepared by reaction of I (M, J = H; other variables as above) with (substituted) (unsatd.) acyl halides, carboxylic acid anhydrides, or carboxylic acid esters in the presence of R1R3NCY(:NR4) (Y = R2, NR2R5; R1-R5 = (substituted) alkyl, alkenyl; R1R2, R3R4 = atoms to form rings). Thus, probucol, succinic anhydride, and DBU were stirred in MeCN at 50° for 1 h to give a mixture comprising probucol monosuccinate 49 weight%, probucol disuccinate 18 weight%, and probucol 33 weight%.

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

TI Process of preparing esters and ethers of probucol and derivatives thereof

AN 2004:610066 CAPLUS

DN 141:156929

TI Process of preparing esters and ethers of probucol and derivatives thereof

IN Weingarten, M. David; Sikorski, James A.

PA Atherogenics, Inc., USA

SO PCT Int. Appl., 136 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

PΙ

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WO		2	A2	20040729	WO 2004-US805				
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CN	1759084		A	20060412	CN 2004-80006265	20040113			
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	2006516569		T 2	20060706	JP 2006-500935	20040113			
					US 2003-439665P	P 20030113			
					WO 2004-US805				

MARPAT 141:156929

give

AB Probucol or a probucol derivative can be efficiently converted to a monoester or monoether of probucol (I) [wherein R1-R4 = H, (un)substituted alkyl; R5, R6 = each (un)substituted alkyl, alkenyl, or aryl; or R5 and R6 can come together to form a carbocyclic ring; X, Y = H, optionally substituted (un)saturated acyl having from 1 to 18 carbon atoms each optionally containing

polar or charged functionality] by reacting the free hydroxyl-containing probucol or a derivative thereof (by which is meant a probucol compound with at least one substituent that is different from that on the parent probucol mol. but which maintains the two free hydroxyl groups), i.e., I (X = Y = H; R1-R6 = same as above), with a Grignard reagent or a lithium reagent that produces a magnesium bromide or lithium salt of probucol or the probucol derivative. The probucol compound anion is then reacted with an ester or ether forming compound. Thus, in a dry 25 mL 3-neck round bottom flask fitted with a reflux condenser, nitrogen inlet, thermocouple and stir bar was charged probucol (0.25 g, 0.48 mmol) followed by 2.5 mL anhydrous toluene and then isopropylmagnesium chloride (0.51 mL, 2.0 M in THF) in 1 portion. The reaction was brought to room temperature and then succinic anhydride (0.25 g, 2.5 mmol) was added in 1 portion. After aging for 45 min, the reaction was slowly quenched with 1 N HCl and diluted with EtOAc. The biphasic reaction was then cooled to room temperature and the phases were separated to

an organic layer containing 60% probucol monosuccinate, 13% probucol disuccinate,

and 27% probucol according to HPLC anal.

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